

## Short Summary of IUPAC Nomenclature of Organic Compounds

### Introduction

The purpose of the IUPAC system of nomenclature is to establish an international standard of naming compounds to facilitate communication. The goal of the system is to give each structure a unique and unambiguous name, and to correlate each name with a unique and unambiguous structure.

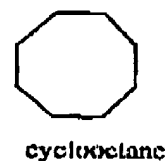
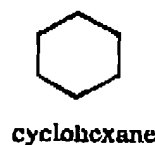
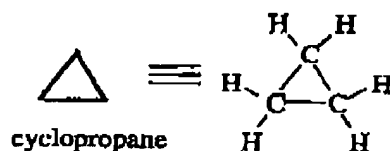
### I. Fundamental Principle

IUPAC nomenclature is based on naming a molecule's longest chain of carbons connected by single bonds, whether in a continuous chain or in a ring. All deviations, either multiple bonds or atoms other than carbon and hydrogen, are indicated by prefixes or suffixes according to a specific set of priorities.

### II. Alkanes and Cycloalkanes

Alkanes are the family of saturated hydrocarbons, that is, molecules containing carbon and hydrogen connected by single bonds only. These molecules can be in continuous chains (called linear or acyclic), or in rings (called cyclic or alicyclic). The names of alkanes and cycloalkanes are the root names of organic compounds. Beginning with the five-carbon alkane, the number of carbons in the chain is indicated by the Greek or Latin prefix. Rings are designated by the prefix "cyclo". (In the geometrical symbols for rings, each apex represents a carbon with the number of hydrogens required to fill its valence.)

$\text{CH}_4$	methane	$\text{CH}_3[\text{CH}_2]_{10}\text{CH}_3$	dodecane
$\text{CH}_3\text{CH}_3$	ethane	$\text{CH}_3[\text{CH}_2]_{11}\text{CH}_3$	tridecane
$\text{CH}_3\text{CH}_2\text{CH}_3$	propane	$\text{CH}_3[\text{CH}_2]_{12}\text{CH}_3$	tetradecane
$\text{CH}_3[\text{CH}_2]_2\text{CH}_3$	butane	$\text{CH}_3[\text{CH}_2]_{18}\text{CH}_3$	icosane
$\text{CH}_3[\text{CH}_2]_3\text{CH}_3$	pentane	$\text{CH}_3[\text{CH}_2]_{19}\text{CH}_3$	heneicosane
$\text{CH}_3[\text{CH}_2]_4\text{CH}_3$	hexane	$\text{CH}_3[\text{CH}_2]_{20}\text{CH}_3$	docosane
$\text{CH}_3[\text{CH}_2]_5\text{CH}_3$	heptane	$\text{CH}_3[\text{CH}_2]_{21}\text{CH}_3$	tricosane
$\text{CH}_3[\text{CH}_2]_6\text{CH}_3$	octane	$\text{CH}_3[\text{CH}_2]_{28}\text{CH}_3$	triacontane
$\text{CH}_3[\text{CH}_2]_7\text{CH}_3$	nonane	$\text{CH}_3[\text{CH}_2]_{29}\text{CH}_3$	hentriacontane
$\text{CH}_3[\text{CH}_2]_8\text{CH}_3$	decane	$\text{CH}_3[\text{CH}_2]_{38}\text{CH}_3$	tetracontane
$\text{CH}_3[\text{CH}_2]_9\text{CH}_3$	undecane	$\text{CH}_3[\text{CH}_2]_{48}\text{CH}_3$	pentacontane



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**III. Nomenclature of Molecules Containing Substituents and Functional Groups**

**A. Priorities of Substituents and Functional Groups**  
 LISTED HERE FROM HIGHEST TO LOWEST PRIORITY, except that the substituents within Group C have equivalent priority.

**Group A—Functional Groups Indicated By Prefix Or Suffix**

<u>Family of Compound</u>	<u>Structure</u>	<u>Prefix</u>	<u>Suffix</u>
Carboxylic Acid	$\text{R}-\overset{\text{O}}{\underset{\text{  }}{\text{C}}}-\text{OH}$	carboxy-	-oic acid (-carboxylic acid)
Aldehyde	$\text{R}-\overset{\text{O}}{\underset{\text{  }}{\text{C}}}-\text{H}$	oxo- (formyl)	-al (carbaldehyde)
Ketone	$\text{R}-\overset{\text{O}}{\underset{\text{  }}{\text{C}}}-\text{R}$	oxo-	-one
Alcohol	$\text{R}-\text{O}-\text{H}$	hydroxy-	-ol
Amine	$\text{R}-\text{N} \begin{array}{l} \diagup \\ \diagdown \end{array}$	amino-	-amine

**Group B—Functional Groups Indicated By Suffix Only**

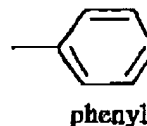
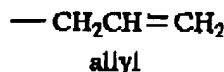
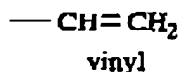
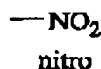
<u>Family of Compound</u>	<u>Structure</u>	<u>Prefix</u>	<u>Suffix</u>
Alkene	$\begin{array}{c} \diagup \quad \diagdown \\ \text{C}=\text{C} \\ \diagdown \quad \diagup \end{array}$	-----	-ene
Alkyne	$-\text{C}\equiv\text{C}-$	-----	-yne

**Group C—Substituents Indicated by Prefix Only**

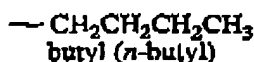
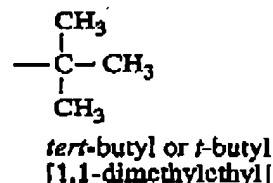
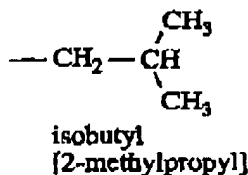
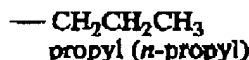
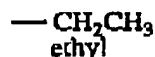
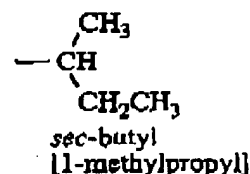
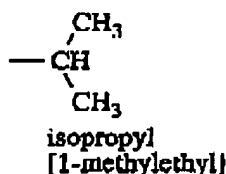
<u>Substituent</u>	<u>Structure</u>	<u>Prefix</u>	<u>Suffix</u>
Alkyl (see list below)	$\text{R}-$	alkyl-	-----
Alkoxy	$\text{R}-\text{O}-$	alkoxy-	-----
Halogen	$\text{F}-$	fluoro-	-----
	$\text{Cl}-$	chloro-	-----
	$\text{Br}-$	bromo-	-----
	$\text{I}-$	iodo-	-----

Group C continued on next page

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**Group C—Substituents, continued**Miscellaneous substituents and their prefixes

Common alkyl groups—replace “ane” ending of alkane name with “yl”. Alternate names for complex substituents are given in brackets.

**B. Naming Substituted Alkanes and Cycloalkanes—Group C Substituents Only**

1. Organic compounds containing substituents from Group C are named following this sequence of steps, as indicated on the examples below:

•Step 1. Find the longest continuous carbon chain. Determine the root name for this parent chain. In cyclic compounds, the ring is usually considered the parent chain, unless it is attached to a longer chain of carbons; indicate a ring with the prefix “cyclo” before the root name. (When there are two longest chains of equal length, use the chain with the greater number of substituents.)

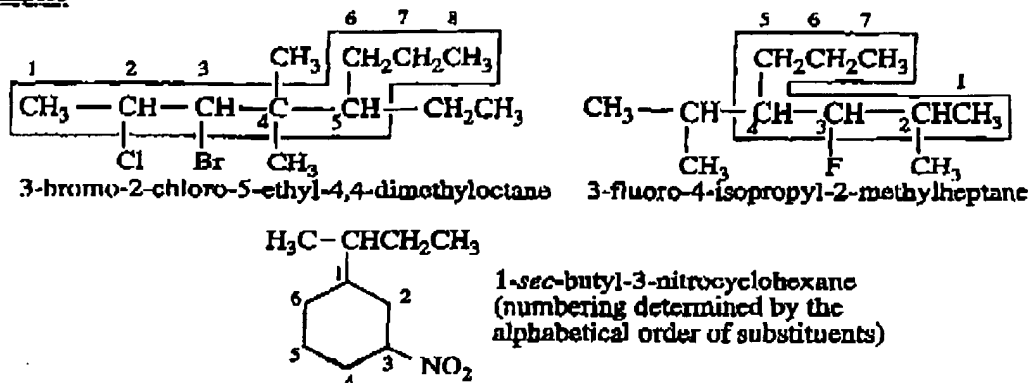
•Step 2. Number the chain in the direction such that the position number of the first substituent is the smaller number. If the first substituents from either end have the same number, then number so that the second substituent has the smaller number, *etc.*

•Step 3. Determine the name and position number of each substituent. (A substituent on a nitrogen is designated with an “N” instead of a number; see Section III.D.1. below.)

•Step 4. Indicate the number of identical groups by the prefixes di, tri, tetra, *etc.*

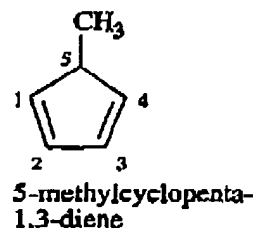
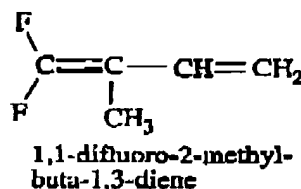
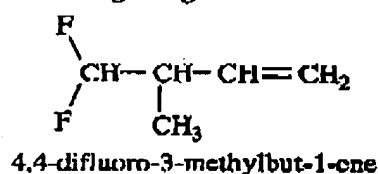
•Step 5. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like *sec-*, *tert-*, *di*, *tri*, *etc.*, but include *iso* and *cyclo*. Always include a position number for each substituent, regardless of redundancies.

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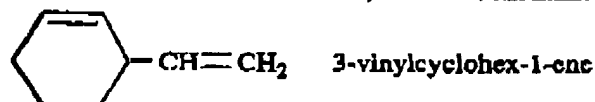
ExamplesC. Naming Molecules Containing Functional Groups from Group B—Suffix Only

## 1. Alkenes—Follow the same steps as for alkanes, except:

- Number the chain of carbons *that includes the C=C* so that the C=C has the lower position number, since it has a higher priority than any substituents;
- Change “ane” to “ene” and assign a position number to the first carbon of the C=C;
- Designate geometrical isomers with a *cis,trans* or *E,Z* prefix.



Special case: When the chain cannot include the C=C, a substituent name is used.

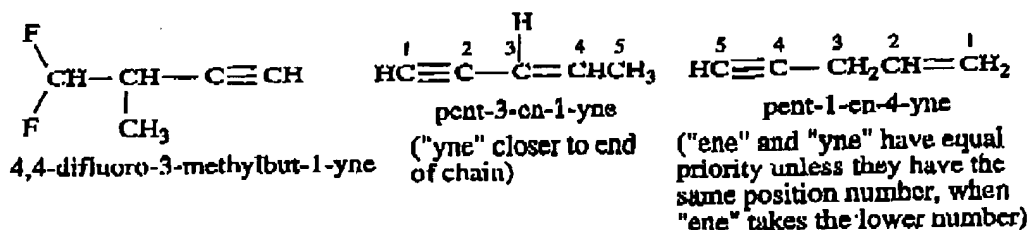


## 2. Alkynes—Follow the same steps as for alkanes, except:

- Number the chain of carbons *that includes the C≡C* so that the functional group has the lower position number;
- Change “ane” to “yne” and assign a position number to the first carbon of the C≡C.

Note: The Group B functional groups (alkene and alkyne) are considered to have equal priority: in a molecule with both a double and a triple bond, whichever is closer to the end of the chain determines the direction of numbering. In the case where each would have the same position number, the double bond takes the lower number. In the name, “ene” comes before “yne” because of alphabetization. See examples on next page.

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(Notes: 1. An "e" is dropped if the letter following it is a vowel: "pent-3-en-1-yne", not "3-pent-3-ene-1-yne". 2. An "a" is added if inclusion of di, tri, etc., would put two consonants consecutively: "buta-1,3-diene", not "but-1,3-diene".)

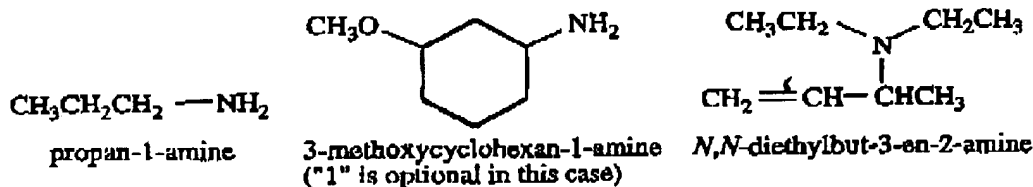
## D. Naming Molecules Containing Functional Groups from Group A—Prefix or Suffix

In naming molecules containing one or more of the functional groups in Group A, the group of highest priority is indicated by suffix; the others are indicated by prefix, with priority equivalent to any other substituents. The table in Section III.A. defines the priorities; they are discussed below in order of increasing priority.

Now that the functional groups and substituents from Groups A, B, and C have been described, a modified set of steps for naming organic compounds can be applied to all simple structures:

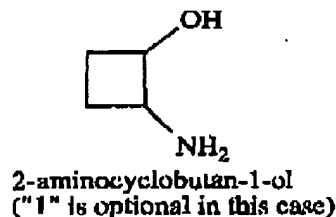
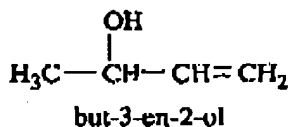
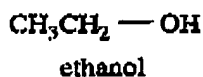
- Step 1. Find the highest priority functional group. Determine and name the longest continuous carbon chain that includes this group.
- Step 2. Number the chain so that the highest priority functional group is assigned the lower number.
- Step 3. If the carbon chain includes multiple bonds (Group B), replace "ane" with "ene" for an alkene or "yne" for an alkyne. Designate the position of the multiple bond with the number of the first carbon of the multiple bond.
- Step 4. If the molecule includes Group A functional groups, replace the last "e" with the suffix of the highest priority functional group, and include its position number.
- Step 5. Indicate all Group C substituents, and Group A functional groups of lower priority, with a prefix. Place the prefixes, with appropriate position numbers, in alphabetical order before the root name.

1. Amines: prefix: amino-; suffix: -amine—substituents on nitrogen denoted by "N"

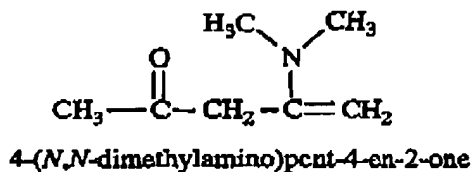
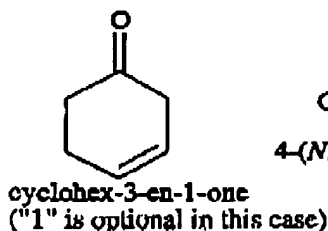
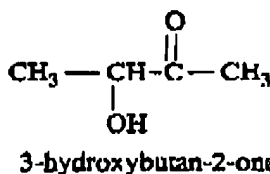
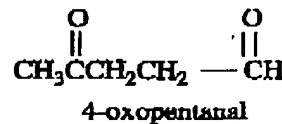
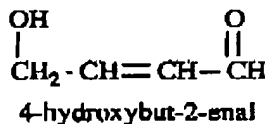
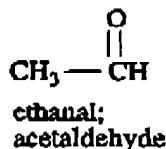
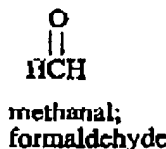


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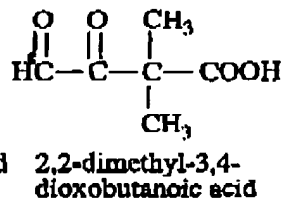
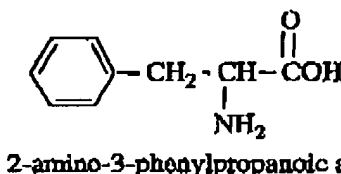
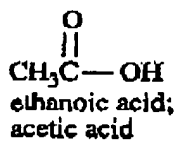
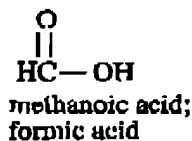
## 2. Alcohols: prefix: hydroxy-; suffix: -ol



## 3. Ketones: prefix: oxo-; suffix: -one

4. Aldehydes: prefix: oxo-, or formyl- ( $\text{O}=\text{CH}-$ ); suffix: -al (abbreviation:  $-\text{CHO}$ ).  
An aldehyde can only be on carbon 1, so the "1" is generally omitted from the name.

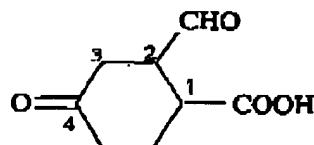
Special case: When the chain cannot include the carbon of the  $\text{CHO}$ , the suffix "carbaldehyde" is used:

5. Carboxylic Acids: prefix: carboxy-; suffix: -oic acid (abbreviation:  $-\text{COOH}$ ).  
A carboxylic acid can only be on carbon 1, so the "1" is generally omitted from the name.

(Note: Chemists traditionally use, and IUPAC accepts, the names "formic acid" and "acetic acid" in place of "methanoic acid" and "ethanoic acid".)

Special case: When the chain numbering cannot include the carbon of the  $\text{COOH}$ , the suffix "carboxylic acid" is used. See example on next page.

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2-formyl-4-oxocyclohexanecarboxylic acid  
("formyl" is used to indicate an aldehyde as a substituent when its carbon cannot be in the chain numbering)

**E. Naming Carboxylic Acid Derivatives**

The six common groups derived from carboxylic acids are salts, anhydrides, esters, acyl halides, amides, and nitriles. Salts and esters are most important.

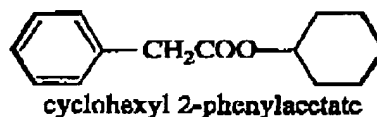
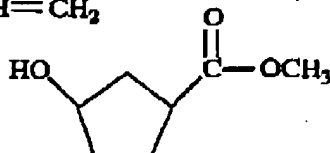
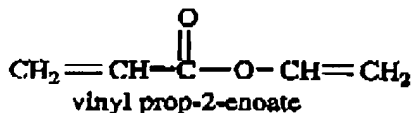
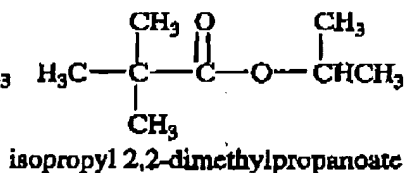
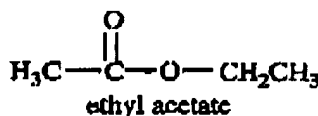
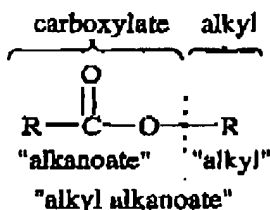
**1. Salts of Carboxylic Acids**

Salts are named with cation first, followed by the anion name of the carboxylic acid, where "ic acid" is replaced by "ate";

acetic acid	becomes	acetate
butanoic acid	becomes	butanoate
cyclohexanecarboxylic acid	becomes	cyclohexanecarboxylate

**2. Esters**

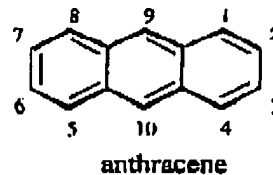
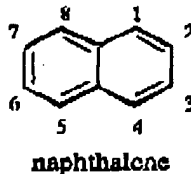
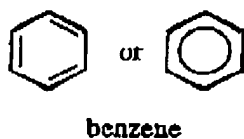
Esters are named as "organic salts" that is, the alkyl name comes first, followed by the name of the carboxylate anion. (common abbreviation:  $-\text{COOR}$ )

**IV. Nomenclature of Aromatic Compounds**

"Aromatic" compounds are those derived from benzene and similar ring systems. As with aliphatic nomenclature described above, the process is: determining the root name of the parent ring; determining priority, name, and position number of substituents; and assembling the name in alphabetical order. *Functional group priorities are the same in aliphatic and aromatic nomenclature.*

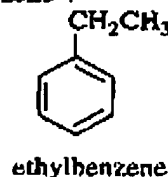
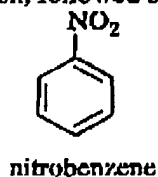
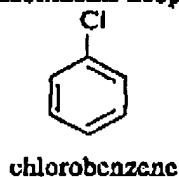
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## A. Common Parent Ring Systems

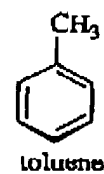
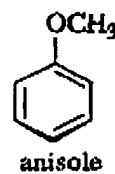
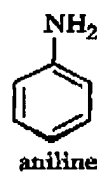
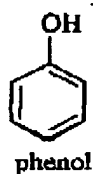
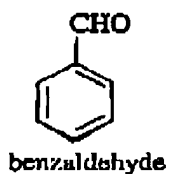
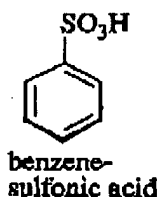
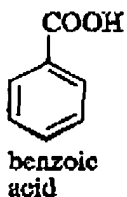


## B. Monosubstituted Benzenes

1. Most substituents keep their designation, followed by the word "benzene":

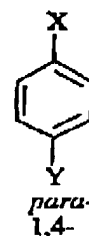
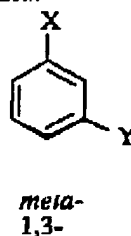
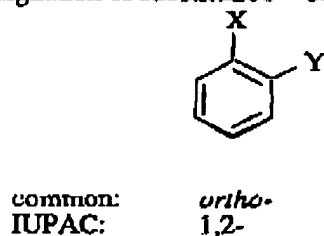


2. Some common substituents change the root name of the ring. IUPAC accepts these as root names, listed here in decreasing priority:

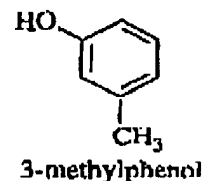
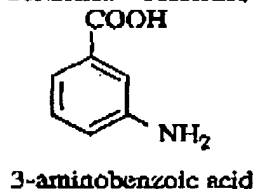
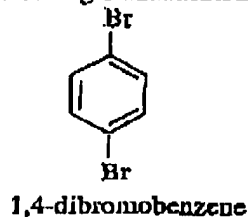


## C. Disubstituted Benzenes

1. Designation of substitution—only three possibilities:



2. Naming disubstituted benzenes—Priorities determine root name and substituents



## IUPAC Recommendations on Macromolecular (Polymer) Nomenclature

### Guide for Authors of Papers and Reports in Polymer Science and Technology

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This Guide is easy to follow and a less formal approach to macromolecular nomenclature than the official IUPAC recommendations, all of which had been previously published in *Pure and Applied Chemistry*.

It has been the goal of the IUPAC Commission on Macromolecular Nomenclature to improve communication between polymer scientists by recommending unambiguous, standardized, and universally understood names and structure representations of polymers.

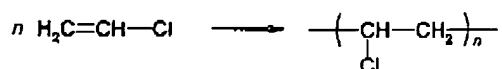
#### A. International Union of Pure and Applied Chemistry (IUPAC) Recommendations

A substance referred to as "a polymer" is different from a low-molecular-weight or "non-polymeric" substance in that usually it has no uniform structure; rather, it consists of a mixture of individual macromolecules. Each macromolecule has a different structural arrangement and length from the others in the mixture. These differences arise from such features as irregularity in monomeric unit sequences within chains, branching irregularities, monomeric unit orientation, and end-group structure.

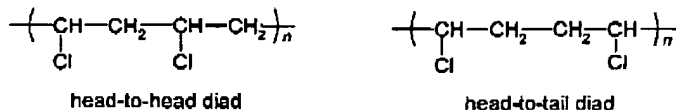
For all types of polymers – single-strand organic, double-strand organic, single-strand inorganic, and coordination – the nomenclature guidelines usually apply to structural representations that are idealized or theoretical; considerations of chain branching, imperfections, or irregularities are excluded.

Because of these problems, attempts to define polymeric substances rigorously are impractical; graphical representation and nomenclature of polymers therefore require a different approach. Naming a polymer of partly known or unknown structure by the "structure-based nomenclature system" may be difficult or impossible unless assumptions are made; naming it by the "source-based nomenclature system" may be possible, however. (Source-based and structure-based nomenclature systems are described below.)

A reaction involving polymerization of a monomer such as vinyl chloride is generally depicted<sup>1</sup> as



The graphical representation of the polymer is ideal rather than true; it contains no information that the polymer contains macromolecules (individual chains) of different chain lengths, and it assumes that all the repeating units are connected in an identical fashion, namely "head-to-tail". In a real polymer, each macromolecule will contain some "head-to-head" diads and some "tail-to-tail" diads.



The precise sequence in each macromolecule of head-to-head, head-to-tail, and tail-to-tail repeating units is usually unknown.

This problem applies also to copolymers; each asymmetric comonomer that can give rise to asymmetric repeating units in a chain adds to the complexity. Each repeating unit can be oriented more than one way in a chain, and also the order of repeating units from comonomers can vary within a chain. For example, the copolymer from the two comonomers 1-propene and 1-butene contains two constitutional or monomeric units:



These can be combined to give several types of copolymers such as alternating, block, graft, periodic, random, statistical, or unspecified.

For these situations, source-based nomenclature is used, which circumvents these problems. A discussion of source-based and structure-based nomenclature systems follows.

#### A1. IUPAC Recommendations for Source-Based Nomenclature

##### A1.1. Nomenclature for Homopolymers

A homopolymer, as the name indicates, is a polymer obtained from only one type of monomer. This may be either an actual monomer, e.g. a reactant, or a hypothetical monomer; an example of the latter is a homopolymer formed by modifying another homopolymer.

Homopolymers are named by writing the prefix "poly", followed by the name of the actual or hypothetical monomer. Names of monomers having substituents or comprising at least two words are parenthesized. Some examples are given in Table 1.

Table 1. Examples of Homopolymer Names

Polymer Name	Polymer Name	Polymer Name	Polymer Name
polyacrylonitrile	poly(1,1-difluoroethylene)	poly(methacrylic acid)	poly(vinyl alcohol)
poly( <i>p</i> -bromostyrene)	poly(ethyl acrylate)	poly(propyl vinyl ether)	poly(vinyl fluoride)
polybut-1-ene	polyethylcnc	poly(vinyl acetate)	poly(vinylidene fluoride)

When multiple sets of parentheses or brackets are needed, IUPAC recommends the use of curved brackets (parentheses) for the innermost application, then square brackets, then curly brackets. These are applied in a "cyclical" pattern, i.e., (...), [...], {[...]}, {{{...}}}, {{{{...}}}}, etc. In contrast, Chemical Abstracts Service (CAS) uses curved brackets (parentheses) for the innermost application and square brackets for all others, i.e. (...), [...], [[...]], etc. This CAS bracketing style is sometimes used with IUPAC-style names, although it has not been officially sanctioned by IUPAC.

Except for polyethylene, all the homopolymers in Table 1 form asymmetrical constitutional units, and the orientation of each constitutional unit within a chain is generally unknown. Furthermore, different samples of any given homopolymer represented by the same constitutional unit can exhibit different chemical and physical characteristics, e.g. average molecular weight or molecular weight distribution.

##### A1.2. Nomenclature for Copolymers

Any polymer derived from more than one type of monomer is usually referred to colloquially as a copolymer.<sup>2</sup> As in the case of homopolymers, each comonomer may be an actual monomer, e.g. a reactant, or a hypothetical monomer.

Copolymers are named by writing the prefix "poly", followed by the names of the actual or hypothetical monomers; an infix, called a connective, is placed between them that indicates the type of sequential arrangement of the constitutional units within the chains.

Table 2 lists the seven types of connectives used to indicate the sequence arrangement of constitutional units; examples of copolymer names are given in Table 3.

Table 2. IUPAC Source-Based Copolymer Classification

Polymer Type	Connective	Example
Unspecified or unknown	-co-	poly(A-co-B)
Random (obeys Bernoullian distribution)	-ran-	poly(A-ran-B)
Statistical (obeys known statistical laws)	-stat-	poly(A-stat-B)
Alternating (for two monomeric units)	-alt-	poly(A-alt-B)

Periodic (ordered sequence for >2 monomeric units)	<i>-per-</i>	poly(A- <i>per</i> -B- <i>per</i> -C)
Block (linear block arrangement)	<i>-block-</i>	polyA- <i>block</i> -polyB
Graft (side chains connected to main chains)	<i>-graft-</i>	polyA- <i>graft</i> -polyB

**Table 3. Examples of Source-Based Copolymer Nomenclature**

Polymer name	Polymer name
Poly(propene- <i>co</i> -methacrylonitrile)	Polyacrylonitrile- <i>block</i> -polybutadiene- <i>block</i> -polystyrene
Poly[(acrylic acid)- <i>ran</i> -(ethyl acrylate)]	Poly[(ethylene oxide)- <i>per</i> -(ethylene oxide)- <i>per</i> -tetrahydrofuran]
Poly(butene- <i>star</i> -ethylene- <i>star</i> -styrene)	Polyisoprene- <i>graft</i> -poly(methacrylic acid)
Poly[(sebacic acid)- <i>alt</i> -butanediol]	

Table 3 contains examples of common or semi-systematic names of comonomers. The systematic names of comonomers may also be used; thus, the polyacrylonitrile-*block*-polybutadiene-*block*-polystyrene polymer in Table 3 may also be named poly(prop-2-enenitrile)-*block*-polybuta-1,3-diene-*block*-poly(ethenylbenzene). IUPAC does not require alphabetized names of comonomers within a polymer name; many names are thus possible for some copolymers.

IUPAC also recommends an alternative scheme for naming copolymers that comprises use of:

1. "copoly" as a prefix, followed by the names of the comonomers
2. an oblique stroke (a solidus) to separate comonomer names
3. addition before "copoly" of any applicable connectives listed in Table 2 except *-co-*.

Table 4 gives the same examples shown in Table 3 but with the alternative format. Comonomer names need not be parenthesized.

**Table 4. Examples of Source-Based Copolymer Nomenclature (Alternative Format)**

Polymer name
copoly(propene/methacrylonitrile)
<i>ran</i> -copoly(acrylic acid/ethyl acrylate)
<i>star</i> -copoly(butene/ethylene/styrene)
<i>alt</i> -copoly(sebacic acid/butanediol)
<i>block</i> -copoly(acrylonitrile/butadiene/styrene)
<i>per</i> -copoly(ethylene oxide/ethylene oxide/tetrahydrofuran)
<i>graft</i> -copoly(isoprene/methacrylic acid)

### A1.3. Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies

A 1997 IUPAC document<sup>2</sup> covers source-based nomenclature for non-linear macromolecules, such as branched, comb, cyclic, graft, network, and star polymers, and macromolecular assemblies, such as interpenetrating polymer networks, polymer blends, and polymer-polymer complexes. The types of polymers in these classes, together with their connectives, are given in Table 5; the terms shown may be used as connectives, prefixes, or both to designate the features present.

**Table 5. Connectives for Non-Linear Macromolecules and Macromolecular Assemblies**

Type	Connective	Type	Connective
Branched (type unspecified)	<i>branch</i>	Network	<i>net</i>
Branched with branch point of functionality f	<i>f-branch</i>	Polymer blend	<i>blend</i>
Comb	<i>comb</i>	Polymer-polymer complex	<i>compl</i>
Cross-link	<i>v</i> (Greek nu)	Semi-interpenetrating polymer network	<i>sipn</i>
Cyclic	<i>cyclo</i>	Short-chain branched	<i>sh-branch</i>
Interpenetrating polymer network	<i>ipn</i>	Star	<i>star</i>
Long-chain branched	<i>l-branch</i>	Star with f arms	<i>f-star</i>

Non-linear polymers are named by using the italicized connective as a *prefix* to the source-based name of the polymer component or components to which the prefix applies; some examples are listed in Table 6.

**Table 6. Examples of Connectives Used as Prefixes for Non-Linear Macromolecules**

Polymer Name	Polymer Structural Features
Poly(acrylic acid)- <i>comb</i> -polyacrylonitrile	Comb polymer with a poly(acrylic acid) backbone and polyacrylonitrile arms
<i>Comb</i> -poly[ethylene- <i>stat</i> -(vinyl chloride)]	Comb polymer with unspecified backbone composition and statistical ethylene/vinyl chloride copolymer arms
Polybutadiene- <i>comb</i> -(polyethylene; polypropene)	Comb polymer with butadiene backbone and arms of polyethene and polypropene
<i>Star</i> -(polyA; polyB; polyC; polyD)	Star polymer with every arm containing comonomers A, B, C, and D
<i>Star</i> -(polyA- <i>block</i> -polyB- <i>block</i> -polyC)	Star polymer with every arm comprising a tri-block segment containing comonomers A, B, and C
<i>Star</i> -poly(ethylene oxide)	A star polymer prepared from ethylene oxide
6- <i>star</i> -poly(ethylene oxide)	A 6-arm star polymer prepared from ethylene oxide
<i>Star</i> -(polyacrylonitrile; polyethylene) ( $M_f$ 20000; 50000)	A star polymer containing polyacrylonitrile arms of MW 20000 and polyethylene arms of MW 50000

Macromolecular assemblies held together by forces other than covalent bonds are named by inserting the appropriate italicized connective between names of individual components; Table 7 gives examples.

**Table 7. Examples of Connectives Used for Polymer Blends and Nets**

Polymer Name
polyethylene- <i>blend</i> -polybutene
poly(methacrylic acid)- <i>blend</i> -poly(methyl methacrylate)
<i>net</i> -poly(4-methylstyrene- <i>μ</i> -divinylbenzene)
<i>net</i> -poly(styrene- <i>alt</i> -(maleic anhydride))- <i>μ</i> -(polyethylene glycol; polypropylene glycol)
<i>net</i> -poly(ethyl acrylate)- <i>spn</i> -polyethylene
[ <i>net</i> -poly(butadiene- <i>stat</i> -4-ethylstyrene)]- <i>ipn</i> -[ <i>net</i> -poly(4-ethylstyrene- <i>μ</i> -divinylbenzene)]

## A2. IUPAC Recommendations for Structure-Based Nomenclature

### A2.1. Nomenclature for Regular Single-Strand Organic Polymers

Regular, single-strand organic polymers consisting of one type of constitutional repeating unit (CRU) in a single sequential unit are named:

poly(constitutional repeating unit)

The complete repeating group is named as a bivalent organic group according to IUPAC recommendations for naming organic compounds.<sup>4</sup> Each CRU comprises one or more subunits, each of which may carry substituents; some examples of subunits are given in Table 8.

**Table 8. Examples of Bivalent Moieties Typically Used as Constitutional Subunits<sup>a</sup>**

Name	Structure	Name	Structure
1-bromoethylene		1-methylethane-1,1-diyl <sup>b</sup>	
butane-1,4-diyl		1-oxoethane-1,2-diyl	
1-(chloromethyl)ethylene		oxy	
cyclohexane-1,2-diyl		1,2-phenylene <sup>c</sup>	

dimethylsilanediyl	$\text{H}_3\text{C}-\text{Si}-\text{CH}_3$	piperazine-1,4-diyl	
ethane-1,1-diyl <sup>b</sup>	$\begin{array}{c} -\text{CH}- \\   \\ \text{CH}_3 \end{array}$	propylimino	$\begin{array}{c} -\text{N}- \\   \\ \text{CH}_2-\text{CH}_2-\text{CH}_3 \end{array}$
ethene-1,2-diyl <sup>c</sup>	$-\text{CH}=\text{CH}-$	pyridine-3,5-diyl	
ethylene	$-\text{CH}_2-\text{CH}_2-$	silanediyl	$-\text{SiH}_2-$
hydrazo	$-\text{NH}-\text{NH}-$	succinyl <sup>f</sup>	$\begin{array}{c} \text{O} \quad \text{O} \\    \quad    \\ -\text{C}-(\text{CH}_2)_2-\text{C}- \end{array}$
imino	$-\text{NH}-$	sulfanediyl <sup>g</sup>	$-\text{S}-$
methylene	$-\text{CH}_2-$	sulfonyl	$-\text{SO}_2-$

<sup>a</sup>Even when substitution is present, the largest subunit possible is selected for naming. Examples: ethylene is not called "methylenemethylene"; terephthaloyl is not called "carbonyl-*p*-phenylenecarbonyl";  $-\text{CH}_2-\text{CO}-\text{CH}_2-\text{CH}_2-$  is called 2-oxobutane-1,4-diyl, not "methylenecarbonylethylene".

<sup>b</sup>IUPAC no longer recommends ethylidene as a name for this subunit when it is connected to two different atoms.

<sup>c</sup>IUPAC still permits vinylene as a name for this subunit, but ethene-1,2-diyl is preferred.

<sup>d</sup>IUPAC no longer recommends isopropylidene as a name for this subunit.

<sup>e</sup>Both *o*-phenylene and 1,2-phenylene are permitted; IUPAC similarly permits both *m*-phenylene and 1,3-phenylene, and both *p*-phenylene and 1,4-phenylene.

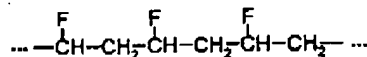
<sup>f</sup>Other similar subunit names permitted include adipoyl, glutaryl, isophthaloyl, malonyl, oxalyl, phthaloyl, and terephthaloyl.

<sup>g</sup>IUPAC still permits thio as a name for this subunit, but sulfanediyl is preferred.

Before a CRU can be named, it must be identified (i.e. the subunits of which it is comprised must be determined); and it must be oriented i.e., written in a manner that follows the guidelines developed by both IUPAC<sup>4</sup> and CAS.<sup>5</sup> IUPAC uses "poly(constitutional repeating unit)" or poly(CRU), whereas CAS names a polymer as "poly(structural repeating unit)" or poly(SRU); the two terms are virtually identical. The nomenclature principles devised by CAS and IUPAC are nearly identical, but names of CRUs (or SRUs) derived by the two organizations are sometimes different because CAS and IUPAC use different names for some subunits. The isopropylidene subunit is a commonly encountered example: CAS names it 1-methylethylidene whereas IUPAC names it 1-methylethane-1,1-diyl.

For most polymer structures, the CRU can be written in more than one way.

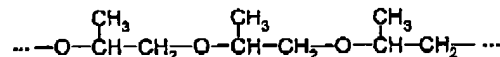
**Example 1:** in a simple polymer, such as



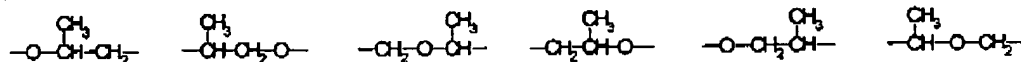
there are two CRUs:



**Example 2:** in a more complex polymer, such as



there are six CRUs:



In Example 1, one of the two CRUs must be selected as the preferred one; similarly, in Example 2, one of the six CRUs must be selected as the preferred one. In each example, the preferred CRU must then be oriented before it can be named correctly.

The complete process of identifying, orienting, and naming a CRU involves three steps, which must be carried out in the order listed:

**Step A: Identifying** the CRU: this is best achieved by drawing an extended segment of the chain that contains at least two constitutional repeating units.

**Step B: Orienting** the CRU: this is the most challenging step. Guidelines are given below for most types of CRU, but comprehensive coverage of all the guidelines is outside the scope of this article.

**Step C: Naming** the complete CRU: the CRU oriented in Step B is named as a bivalent organic group according to the usual nomenclature guidelines for organic chemistry.

The guidelines presented below were designed to enable determination of: (1) *seniority* among subunits, i.e., which subunit is written leftmost in the complete CRU; and (2) the *direction* along the chain in which to continue to the end of the CRU.

**(1) Seniority**

Among the bivalent subunits that comprise a single-strand CRU, the order of seniority is:

**Subunit type (a):** moieties comprising heterocycles

Examples: piperidine-3,5-diyl  
thiophene-2,5-diyl

**Subunit type (b):** hetero-atomic acyclic moieties

Examples: imino  
oxy  
sulfanediyl  
sulfonyl

**Subunit type (c):** moieties comprising carbocycles

Examples: 1,3-phenylene  
cyclohexane-1,3-diyl

**Subunit type (d):** moieties comprising carbon chains

Examples: 1-chloroethylene  
propane-1,3-diyl

Seniority within subunit types (a) - (d) is determined by further guidelines:

**Subunit type (a):** heterocycles. A nitrogen-containing ring system is senior to a ring system containing a hetero atom other than nitrogen.<sup>4,6</sup> Further descending order of seniority is determined by:

- (i) the highest number of rings in the ring system
- (ii) the largest individual ring in the ring system
- (iii) the largest number of hetero atoms
- (iv) the greatest variety of hetero atoms

**Subunit type (b):** hetero-atomic acyclic moieties. The senior bivalent subunit is the one nearest the top, right-hand corner of the periodic table; the order is: O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg.

**Subunit type (c):** carbocyclic moieties. Seniority<sup>4</sup> is determined by:

- (i) the highest number of rings in the ring system
- (ii) the largest individual ring in the ring system
- (iii) degree of ring saturation; an unsaturated ring is senior to a saturated ring of the same size

**Example 3:** A 3-ring system is senior to a 2-ring system.

**Example 4:** A 2-ring system with two 6-membered rings is senior to a 2-ring system with one 6-membered and one 5-membered ring.

**Example 5:** A fused 2-ring system (two atoms common to both rings) is senior to a spiro 2-ring system (one atom common to both rings).<sup>7</sup>

**Subunit type (d):** carbon-containing acyclic groups. Descending order of seniority is determined by:

- (i) chain length (longer is senior to shorter)
- (ii) number of substituents (higher number is senior to lower number)
- (iii) ascending order of locants
- (iv) alphabetical order of names of substituent groups

The seniority guidelines given above are applied only to the subunits of the main chain or backbone. Substituents in main-chain subunits, whether the subunits are of type (a), (b), (c), or (d), do not control CRU selection unless otherwise identical chain subunits need to be differentiated by either the number of substituents or their alphabetical order.

## (2) Direction

The preferred CRU is the one that begins with the subunit of highest seniority and continues along the chain in the direction of either (1) another occurrence of the same subunit or (2) the subunit next in seniority. If, in (1), there is more than one further occurrence of the same subunit, the preferred path is the shorter one between the senior subunit and one of its further occurrences.

**Example 6:** consider the CRU ...C-C-O-C-C-S-C-C-O-C-C-S-C-C-O-C-...

$$\begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \end{array}$$

**Identifying the CRU:** this CRU has a regularly repeating eight-atom sequence. Thus, starting from one sulfur atom and proceeding along the chain in either direction as far as (but not including) the next sulfur atom results in the conclusion that the CRU contains eight atoms. This sequence also contains two oxygen atoms.

**Orienting the CRU:** there are no heterocycles [subunit type (a)] present; therefore one of the heteroatoms [subunit type (b)] must be the senior subunit. O is senior to S (see above), and therefore one of the two oxygen atoms must be selected as senior subunit. Numbering the two oxygen atoms arbitrarily O<sup>1</sup> and O<sup>2</sup> gives:

...C-C-O<sup>1</sup>-C-C-S-C-C-O<sup>2</sup>-C-O<sup>1</sup>-C-C-S-C-C-O<sup>2</sup>-C-...

Beginning with either occurrence of O<sup>1</sup> and proceeding along the chain in the direction of the second subunit of equal seniority, O<sup>2</sup>, as far as (but not including) a second occurrence of O<sup>1</sup>, gives two possibilities, each eight atoms long (for this determination, reading in either direction is permissible):

- (1) -O<sup>1</sup>-C-C-S-C-C-O<sup>2</sup>-C-
- (2) -C-C-S-C-C-O<sup>2</sup>-C-O<sup>1</sup>-

According to the guidelines, the preferred path from O<sup>1</sup> to O<sup>2</sup> is the shorter one; of the two possibilities shown immediately above, therefore, sequence (2), when laterally reversed from -C-C-S-C-C-O<sup>2</sup>-C-O<sup>1</sup>- to -O<sup>1</sup>-C-O<sup>2</sup>-C-C-S-C-C-, becomes the preferred CRU.

The **defined** and **oriented** CRU is thus -O-C-O-C-C-S-C-C-. It may now be **named**:

1. Select the names of its subunits (e.g. from Table 8) in the order in which they occur as the sequence is read from left to right;
2. Write them in the order in which they were selected;
3. Precede the subunit name assembly with poly; use parentheses, brackets, or both, as necessary.

The preferred name for this CRU, written in the style "poly(constitutional repeating unit)", is thus poly(oxyethyleneoxyethylenesulfanedithioethylene); poly(oxyethyleneoxyethylenethioethylene) is an acceptable alternative.

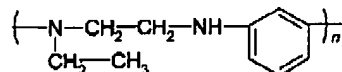
Application of these guidelines to example 2, ...-O-CH(CH<sub>3</sub>)-CH<sub>2</sub>-..., gives the following results:

1. O is the senior subunit
2. For the substituted ethylene subunit, the preferred position for the methyl group is on the leftmost carbon, i.e., it is assigned the lowest possible locant when reading from left to right

The name of the polymer is thus poly[oxy(1-methylethylenc)].<sup>8</sup>

Two more examples are shown to illustrate application of the guidelines.

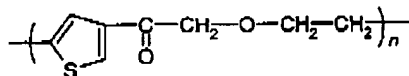
**Example 6:** poly[(ethylimino)ethyleneimino-1,3-phenylene] has the following structure:



The steps that led to this orientation and name were:

1. One of the two nitrogen atoms is the senior subunit.
2. The substituted N is senior to the unsubstituted one [see **subunit type (d)(ii)** above].
3. The shorter path from the senior N to the unsubstituted N is via the ethylene subunit (two atoms between the two N atoms), not via the ring (three atoms between the two N atoms).

**Example 7:** poly[thiophene-2,4-diyl(1-oxoethylene)oxyethylene] has the following structure:



The steps that led to this orientation and name were:

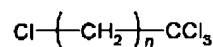
1. The heterocycle is the senior subunit.
2. The path length from the senior subunit to -O-, the next senior subunit, is the same in both directions along the CRU. Guideline **subunit type (d)(ii)** is used to make a decision between the two paths of equal length; the substituted subunit (1-oxoethylene) is senior to the unsubstituted subunit (ethylene).

The procedure for naming end-groups on CRUs is as follows:

1. Identify, orient, and name the CRU per the guidelines above
2. Name the end-groups as substituents; use parentheses, brackets, or both, as necessary
3. Precede the name of the left-hand end-group by the Greek letter  $\alpha$
4. Precede the name of the right-hand end-group by the Greek letter  $\omega$
5. Assemble the complete name in the format:  
 $\alpha$ -(left-hand end-group)- $\omega$ -(right-hand end-group)poly(CRU)

For symmetrical CRUs, e.g. poly(methylene), end-group names are alphabetized; the end-group that alphabetizes first is designated as the  $\alpha$  end-group (see Example 8).

**Example 8:**  $\alpha$ -chloro- $\omega$ -(trichloromethyl)poly(methylene)



For asymmetrical CRUs in which the two end-group names are different from one another, the  $\alpha$ -end-group is cited first, regardless of alphabetic order (see Example 9).

**Example 9:**  $\alpha$ -(trichloromethyl)- $\omega$ -chloropoly(1,1-difluoroethylene)

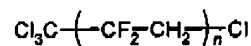
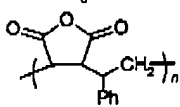
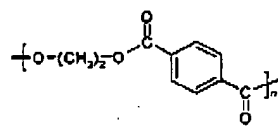
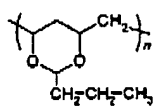


Table 9 compares and contrasts structure-based and source-based names for some common polymers.

**Table 9. Structure-Based, Source-Based, and Trivial Names for Some Common Polymers**

Structure	Structure-Based Names	Source-Based and Trivial Names
	Poly(1-acetoxyethylene)	Poly(vinyl acetate)
	Poly(but-1-ene-1,4-diyl)	Polybutadiene <sup>a</sup>

$\left( \text{CH}(\text{Cl})\text{CH}_2 \right)_n$	Poly(1-chloroethylene)	Poly(vinyl chloride)
$\left( \text{CH}(\text{CN})\text{CH}_2 \right)_n$	Poly(1-cyanoethylene)	Polyacrylonitrile
$\left( \text{CF}_2\text{CH}_2 \right)_n$	Poly(1,1-difluoroethylene)	Poly(vinylidene difluoride)
$\left( \text{CF}_2 \right)_n$	Poly(difluoromethylene) <sup>b</sup>	Poly(tetrafluoroethylene)
$\left( \text{C}(\text{CH}_3)_2\text{CH}_2 \right)_n$	Poly(1,1-dimethylethylene)	Polyisobutylene
	Poly[(2,5-dioxotetrahydrofuran-3,4-diyl)(1-phenylethylene)]	Poly(maleic anhydride- <i>alt</i> -styrene)
$\left( \text{CH}(\text{OH})\text{CH}_2 \right)_n$	Poly(1-hydroxyethylene)	Poly(vinyl alcohol)
$\left[ \text{NH}-\text{C}(=\text{O})-(\text{CH}_2)_4-\text{C}(=\text{O})-\text{NH}-(\text{CH}_2)_6 \right]_n$	Poly(iminoadipoyliminohexane-1,6-diyl)	Poly(adipic acid- <i>alt</i> -hexamethylenediamine); nylon 66; poly(hexamethylene adipamide)
$\left[ \text{NH}-\text{C}(=\text{O})-(\text{CH}_2)_5 \right]_n$	Poly[imino(1-oxohexane-1,6-diyl)]	Poly( $\epsilon$ -caprolactam); nylon 6
$\left[ \text{C}(\text{CH}_3)(\text{CO}_2\text{CH}_3)\text{CH}_2 \right]_n$	Poly[1-(methoxycarbonyl)-1-methylethylene]	Poly(methyl methacrylate)
$\left( \text{CH}_2 \right)_n$	Poly(methylene) <sup>b</sup>	Polyethene; polyethylene
$\left( \text{O}-\text{CH}_2\text{CH}_2 \right)_n$	Poly(oxyethylene)	Poly(oxirane); poly(ethylene oxide)
	Poly(oxyethyleneoxyterephthaloyl)	Poly(ethylene terephthalate); PET
$\left( \text{O}-\text{C}_6\text{H}_4 \right)_n$	Poly(oxy-1,4-phenylene)	Poly(phenylene oxide)
$\left( \text{CH}(\text{CH}_3)\text{CH}_2 \right)_n$	Poly(1-methylethylene)	Polypropylene; polypropene
$\left( \text{CH}(\text{Ph})\text{CH}_2 \right)_n$	Poly(1-phenylethylene)	Poly(ethenylbenzene); polystyrene
	Poly[(2-propyl-1,3-dioxane-4,6-diyl)methylene]	Poly(vinyl butyral)

<sup>a</sup>This assumes polymerization of poly(butadiene) in the so-called "1,4" mode, for which the CRU is usually written  $-\text{[CH}_2\text{-CH=CH-CH}_2\text{]}_n-$ . According to CAS and IUPAC guidelines, this is incorrect; the correct

structure and name are as shown in the Table. Similarly, isoprene polymerized in the so-called "1,4" mode should be depicted as  $-\text{[CH(CH}_3\text{)=CH-CH}_2\text{-CH}_2\text{]}_n-$  and named poly(1-methylbut-1-ene-1,4-diyl).

<sup>b</sup>Structure-based representations  $-(\text{CH}_2)_n-$  and  $-(\text{CF}_2)_n-$  are preferred for poly(methylene) and poly(difluoromethylene), respectively; however, because of past usage and an attempt to retain some similarity to the CRU formulas of homopolymers derived from other ethene derivatives, the CRU representations  $-(\text{CH}_2\text{-CH}_2)_n-$  and  $-(\text{CF}_2\text{-CF}_2)_n-$  are also acceptable.

## A2.2. Nomenclature for Irregular Single-Strand Organic Polymers

The naming of each constitutional unit of an irregular, single-strand organic polymer follows the guidelines in section A2.1 above. The complete polymer name is constructed by combining names of individual constitutional units, separating them with as many solidi (oblique strokes) as necessary, parenthesizing or bracketing the complete expression, and adding the prefix "poly".<sup>3</sup> The solidus is used to indicate that information is unavailable on the individual CRU sequence in the polymer. In graphical representations of these polymers, the hyphens or dashes at each end of each CRU depiction are shown *completely within* the enclosing parentheses; this indicates that they are not necessarily the terminal bonds of the macromolecule. The examples in table 10 illustrate application of these guidelines.

**Table 10. Nomenclature Examples of Irregular Single-Strand Organic Polymers**

Structure	Name
$\left( -\text{CH}=\text{CH}-\text{CH}_2-\text{CH}_2- / \begin{array}{c} \text{CH}-\text{CH}_2 \\   \\ \text{CH}=\text{CH}_2 \end{array} \right)_n$	Poly(but-1-ene-1,4-diyl/1-vinylethylene) Note: depiction of the product from polymerization of buta-1,3-diene in the so-called "1,2-" and "1,4-" modes
$\left( \begin{array}{c} \text{CH}-\text{CH}_2 \\   \\ \text{Cl} \end{array} / \begin{array}{c} \text{CH}-\text{CH}_2 \\   \\ \text{Ph} \end{array} \right)_n$	Poly(1-chloroethylene/1-phenylethylene) Note: representation of a copolymer of vinyl chloride and styrene
$\left( -\text{CH}_2- / \begin{array}{c} \text{Cl} \\   \\ \text{CH} \\   \\ \text{Cl} \end{array} / \begin{array}{c} \text{Cl} \\   \\ \text{C} \\   \\ \text{Cl} \end{array} - \right)_n$	Poly(dichloromethylene/chloromethylene/methylene) Note: representation of the idealized product from chlorination of poly(ethylene), and also from chlorination of poly(vinyl chloride)
$\left( \begin{array}{c} \text{O} \\    \\ \text{O}-\text{C}-\text{CH}_3 \\   \\ \text{CH}-\text{CH}_2 \end{array} / \begin{array}{c} \text{OH} \\   \\ \text{CH}-\text{CH}_2 \end{array} \right)_n$	Poly(1-acetoxyethylene/1-hydroxyethylene) Note: representation of partially hydrolyzed head-to-tail poly(1-acetoxyethylene)
$\left( \begin{array}{c} \text{CH}-\text{CH}_2 \\   \\ \text{OH} \end{array} / \begin{array}{c} \text{CH}-\text{CH}_2 \\   \\ \text{O}-\text{C}-\text{CH}_3 \end{array} / \begin{array}{c} \text{CH}_2 \\   \\ \text{O} \\   \\ \text{CH}_2-\text{CH}_2-\text{CH}_3 \end{array} \right)_n$	Poly[(1-acetoxyethylene)/(1-hydroxyethylene)/[(2-propyl-1,3-dioxane-4,6-diyl)methylene]] Note: representation of poly(vinyl alcohol) partially converted to poly[(vinyl acetate)-co-(vinyl butyral)]

## A2.3. Nomenclature for Regular Double-Strand Organic Polymers

Every macromolecule in a double-strand polymer contains a continuous sequence of rings; there are no single, acyclic bonds. Spiro polymers have one atom in common in adjacent rings. Ladder polymers have two or more atoms in common in adjacent rings. As for linear single-strand polymers, a double-strand polymer CRU must be identified and oriented before the polymer can be named.<sup>6</sup> The CRU is a multivalent group (usually tetravalent) in which attachment to all (usually four) atoms is cited. The CRU is named according to the IUPAC guidelines for organic nomenclature.<sup>4</sup> The polymer is named in the style

poly(constitutional repeating unit)

Since double-strand polymers have no single, acyclic bonds, the CRU can be defined only by breaking rings. When rings are broken, the following guidelines are applied in decreasing order of priority:

**Guideline 1:** Minimize the number of free valencies in the CRU.

**Guideline 2:** Maximize the number of most preferred hetero atoms in the ring system.

**Guideline 3:** Maintain intact the most preferred ring system.<sup>4</sup>

Further decisions are based upon:

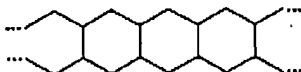
**Guideline 4:** Ring system seniority<sup>4,5</sup>

**Guideline 5:** Orientation of the CRU to place the lowest free-valence locant at the lower-left position of the structural diagram

**Guideline 6:** Placement of any acyclic subunits on the right side of the structural diagram, within the CRU

Three examples are shown to illustrate application of the guidelines.

**Example 10:** For the ladder polymer



comprising adjacent, six-membered, saturated carbon rings, the preferred CRU is an acyclic subunit of four carbon atoms with four free valencies, one at each atom. The lower-left atom is assigned the lowest locant.

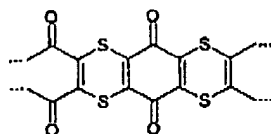


Within the CRU name, the free-valence locants are written immediately before the end of the tetravalent unit to which they apply. The locants are cited clockwise from the lower-right position; thus, they are always cited, complete with punctuation (commas and colon), in the following order and manner:

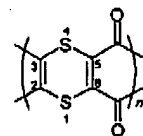
lower-left, upper-left:upper-right, lower-right

The name of this ladder polymer is poly(butane-1,4:3,2-tetrayl).

**Example 11:** For the ladder polymer

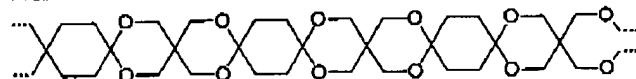


which contains one type of heterocyclic ring that alternates with one type of carbocyclic ring, the heterocyclic ring is senior to the carbocyclic ring (see **Guideline 2** above); therefore the carbocyclic ring is broken, the heterocyclic ring is placed leftmost, and the two acyclic chains resulting from fracture of the carbocyclic ring are placed to the right of the cyclic subunit (see **Guideline 6** above).

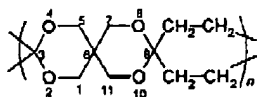


The name of this ladder polymer is poly(1,4-dithiin-2,3:5,6-tetrayl-5,6-dicarbonyl).

**Example 12:** The spiro polymer



contains three-rings – two 1,3-dioxane rings (facing in opposite directions) and a cyclohexane ring. The preferred CRU retains the two 1,3-dioxane rings, and the carbocyclic ring is broken (see **Guideline 2** above). The acyclic fragments are placed to the right of the cyclic subunits (see **Guideline 6** above).



The name of this spiro polymer is poly(2,4,8,10-tetraoxaspiro[5.5]undecane-3,3:9,9-tetra-1,9,9-diethylenc).

#### A2.4. Nomenclature for Regular Single-Strand Inorganic and Coordination Polymers

IUPAC names of inorganic and coordination polymers<sup>10</sup> are based on the fundamental principles of nomenclature developed for organic polymers. The CRU must thus be *defined* and *oriented* before it can be *named*. However, owing to basic differences between inorganic and organic nomenclature, subunits of inorganic CRUs are named as inorganic or coordination groups, which include covalent or coordinate bonding, respectively. The polymer is named by attaching to the name of the CRU a suitable prefix, such as "poly" or "catena".

CRU orientation depends upon *seniorities* of, and preferred *direction* for citation of, each constituent subunit. The principle of coordination nomenclature places emphasis on a coordination centre. The constituent subunit of highest seniority must therefore contain at least one central atom; bridging groups between central backbone atoms have lower seniority. When there are two or more central atoms in the CRU of a linear inorganic or coordination polymer, the senior subunit is the one containing the central atom occurring *latest* in the following atom sequence.<sup>10</sup>

F, Cl, Br, I, At, O, S, Se, Te, Po, N, P, As, Sb, Bi, C, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl, Zn, Cd, Hg, Cu, Ag, Au, Ni, Pd, Pt, Co, Rh, Ir, Fe, Ru, Os, Mn, Tc, Re, Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, La → Lu, Ac → Lr, Be, Mg, Ca, Sr, Ba, Ra, Li, Na, K, Rb, Cs, Fr, He, Ne, Ar, Kr, Xe, Rn.

This seniority order *differs* from that applied to hetero atoms used for organic polymer nomenclature guidelines.<sup>4</sup>

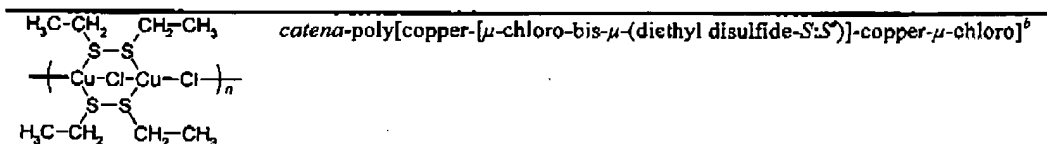
When further choice is necessary for selection of a senior subunit, preference is given, in order, to:

1. A polynuclear coordination centre, in order of decreasing number of central atoms.
2. The central atom or coordination centre with the greatest number of attached coordinating atoms, excluding coordinating atoms of bridging ligands in the polymer chain backbone.
3. The central atom or coordination centre, the name of which (including ligands and any multiplying prefixes other than bridging ligands in the polymer chain backbone) alphabetizes first.

Table 11 gives examples of application of these guidelines.

Table 11. Examples of IUPAC Inorganic Nomenclature

Structure	Name
$\left( \begin{array}{c} \text{CH}_3 \\   \\ \text{---} \text{Sn} \text{---} \\   \\ \text{Ph} \end{array} \right)_n$	catena-poly[methylphenyltin]
$\left( \begin{array}{cc} \text{Cl} & \text{CH}_3 \\   &   \\ \text{---} \text{Si} & \text{---} \text{Si} \text{---} \\   &   \\ \text{Cl} & \text{CH}_3 \end{array} \right)_n$	catena-poly[(dichlorosilicon)(dimethylsilicon)]
$\left( \begin{array}{c} \text{NH}_3 \\   \\ \text{---} \text{Zn} \text{---} \text{Cl} \text{---} \\   \\ \text{Cl} \end{array} \right)_n$	catena-poly[(amminechlorozinc)-μ-chloro] <sup>a</sup>
$\left( \begin{array}{cc} \text{H} & \text{CH}_3 \\   &   \\ \text{---} \text{B} & \text{---} \text{N} \text{---} \\   &   \\ \text{H} & \text{CH}_3 \end{array} \right)_n$	catena-poly[(dihydroboron)-μ-(dimethylamido)] <sup>a</sup>



<sup>a</sup>Many coordination polymers contain a mononuclear central atom with a bridging ligand. CRUs with this type of structure are named by citing (1) the central atom, together with any attached, non-bridging groups, which are cited as a prefix to the central atom; (2) the Greek letter  $\mu$ ; and (3) the bridging ligand name.

<sup>b</sup>Multiple bridging ligands between two central atoms are alphabetized. For bridging ligands, italicized element symbols (separated by a colon) that indicate the coordinating atoms are cited in the direction in which the CRU is read, i.e. left to right.

#### A2.5. Nomenclature for Regular Quasi-Single-Strand Coordination Polymers

CRUs comprising backbones with one mononuclear central atom and two or more bridging ligands (alike or different), or a chelating ligand, are named as follows: (1) cite the name of the central atom, prefixed by the names of its associated non-bridging ligand(s); (2) cite the names of the bridging ligands, each prefixed by the Greek letter  $\mu$ . If there are two or more identical bridging ligands, an appropriate numerical prefix is added to indicate the number.<sup>10</sup> For polymers with identical bridging ligands, the general polymer name format is:

*catena-poly[(associated non-bridging ligands)mononuclear central atom-μ-bridging ligand(s)]*

For two or more non-identical bridging ligands, the names of the ligands are alphabetized:

*catena-poly[(associated non-bridging ligands)mononuclear central atom-μ-bridging ligand a-μ-bridging ligand b]*

Parentheses, brackets, or both, are used as needed. Table 12 shows application of these guidelines.

**Table 12. Nomenclature Examples for Quasi-Single-Strand Coordination Polymers**

Structure	Name	Structure	Name
	<i>catena-poly[palladium-di-μ-chloro]</i>		<i>catena-poly[titanium-tri-μ-chloro]</i>
	<i>catena-poly[silicon-di-μ-thio]</i>		<i>catena-poly[platinum(μ-bromo-μ-chloro)]</i>

#### B. Common, Semi-Systematic, and Trivial Names Usage

Chemical nomenclature's primary goal is to identify chemical substances by their names so that scientists can communicate data about them without the need for representations of chemical structure. Systematic chemical nomenclature systems were designed specifically to enable readers to deduce chemical structures of substances from names. As discussed above, structure-based names of polymers are based on their structural features.

For many frequently used substances, however, traditional names not necessarily related to the chemical structures they represent have existed for over 40 years, and they are still used daily. These traditional names are usually referred to as common, semi-systematic, or trivial names. Provided there is no ambiguity, IUPAC allows continued use of such names, both for polymers and for polymer fragments, moieties, or subunits. IUPAC acknowledges that many common polymers have well established and frequently used semi-systematic or trivial names, and it is not intended that structure-based names should now displace them. Nevertheless, IUPAC encourages minimal use of semi-systematic or trivial polymer names in scientific communications. Examples of semi-systematic or trivial names still permitted include adipoyl, ethylenc, isophthaloyl, malonyl, oxalyl, phthaloyl, succinyl, and terephthaloyl.

Table 13 gives some examples of common, semi-systematic, or trivial monomer names, together with their corresponding IUPAC systematic names. Table 14 lists some examples of common, semi-systematic, or trivial polymer names, together with their IUPAC systematic, structure-based names.

**Table 13. Selected Common Monomers: Common, Semi-Systematic, or Trivial Names vs. IUPAC Structure-Based Names**

Common, Semi-Systematic, or Trivial Names	Typical IUPAC Name <sup>a</sup>
2,2-Bis( <i>p</i> -hydroxyphenyl)propane; bisphenol A; BPA	4,4'-(1-Methylethane-1,1-diyl)diphenol
Bis(4-isocyanatophenyl)methane;	Methylenedi-1,4-phenylene diisocyanate
4,4'-diisocyanatodiphenylmethane;	
4,4'-methylenebis(phenyl isocyanate);	
4,4'-methylenediphenyl diisocyanate; MDI	
Caprolactam	Hexano-6-lactam
1,4-Cyclohexylene diisocyanate; CHDI;	Cyclohexane-1,4-diyl diisocyanate
1,4-diisocyanatocyclohexane	
1,2-Diaminocyclohexane	Cyclohexane-1,2-diamine
Diaminodiphenyl ether; DAPE; ODA; 4,4'-ODA	4,4'-Oxydianiline
1,6-Diisocyanatohexane; HDI; HMDI	Hexane-1,6-diyl diisocyanate
2,4-Diisocyanatotoluene; 2,4-TDI;	4-Methyl-1,3-phenylene diisocyanate
2,4-tolylene diisocyanate	
Ethylene glycol	Ethane-1,2-diol
Hexamethylenediamine; HMD; HMDA	Hexane-1,6-diamine
Isophorone diisocyanate; IPDI	3-(Isocyanatomethyl)-3,5,5-trimethylcyclohexyl isocyanate <sup>b</sup>
Pyromellitic dianhydride; PMDA	Benzene-1,2,4,5-tetracarboxylic dianhydride

<sup>a</sup>IUPAC substance names are always unambiguous, but they are not necessarily unique; a substance may therefore have more than one IUPAC name. Some typical names are given.

The IUPAC name for IPDI is appreciably different from the uninverted CAS name 5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane. This difference arises because IUPAC names IPDI as an ester of isocyanic acid, whereas CAS names it as a substituted cyclohexane (according to CAS 9CI nomenclature, "the -NCO group is not classified as a functional group).

**Table 14. Selected Common Polymers: Common, Semi-Systematic, or Trivial Names vs. IUPAC Structure-Based Names**

Common, Semi-Systematic, or Trivial Names	IUPAC Structure-Based Name
2,2-Bis(4-hydroxyphenyl)propane polycarbonate; bisphenol A polycarbonate	Poly[oxycarbonyloxy-1,4-phenylene(1-methylethane-1,1-diyl)-1,4-phenylene]
Polycaprolactam; polycaproamide; nylon 6	Poly[imino(1-oxohexane-1,6-diyl)]
Polyetherketone; PEK	Poly(oxy-1,4-phenylene-carbonyl-1,4-phenylene)
Poly(ethylene oxide), polyoxyethylene; PEO	Poly(oxyethylene)
Poly(ethylene terephthalate); PET; PETP; PETE <sup>a</sup>	Poly(oxyethyleneoxyterephthaloyl)
Poly(hexamethylene adipamide); nylon 66	Poly(iminoadipoyliminohexane-1,6-diyl)
Poly(phenylene sulfide); poly( <i>p</i> -phenylene sulfide); PPS	Poly(thio-1,4-phenylene)
Poly(tetramethylene oxide); polyoxytetramethylene; PTMO	Poly(oxybutane-1,4-diyl)

<sup>a</sup>In the United States, PETE is frequently stamped on or molded into the bottom of PET bottles for the purpose of classifying or identifying the plastic type during recycling operations.

Abbreviations and acronyms are used widely for both non-polymeric and polymeric substances, as well as for additives, modifiers, and fillers. When creating acronyms, scientists unfortunately rarely consider uniqueness. Thus, AA has been used for both acrylic acid and adipic acid, while AN has been used for both acrylonitrile and ammonium nitrate. To include a list of acronyms here would therefore serve little purpose, because new ones are created daily. IUPAC recommends that every author who writes a chemical publication should define each abbreviation used therein in a list near the beginning of the paper.<sup>13</sup> IUPAC has recommended standard abbreviations for representing polymers.<sup>14</sup> The fourth edition of the *Polymer Handbook* contains a list of commonly used abbreviations recognized by international organizations.<sup>15</sup> Publication titles should cite acronyms or abbreviations only if they are defined within the title. An example is "Preparation of poly(methyl methacrylate) (PMMA)".

### C. Polymer Class Names

Many publications (encyclopedias, handbooks, indexes, textbooks, etc.) that discuss polymer nomenclature group information on polymers under polymer class names. These classes are not mutually exclusive; some are very specific, whereas others are more generic. Table 15 lists most of the terms commonly encountered in such publications.

**Table 15. List of Commonly Encountered Polymer Class Names**

Column 1	Column 2	Column 3	Column 4
Acrylic polymers	Polyarylenes	Polyimidazoles	Polysilazanes
Alkyd resins	Polyazomethines	Polyimides	Polysiloxanes
Aminoplasts	Polybenzimidazoles	Polyimines	Polysilsesquioxanes
Coumarone-indene-resins	Polybenzothiazoles	Polyisocyanurates	Polysulfides
Epoxy resins	Polybenzoxazinones	Polyketones	Polysulfonamides
Fluoropolymers	Polybenzoxazoles	Polyolefins	Polysulfones
Phenolic resins	Polybenzyls	Polyoxadiazoles	Polythiazoles
Polyacetals	Polycarbodiimides	Polyoxides	Polythioalkylenes
Polyacetylenes	Polycarbonates	Polyoxyalkylenes	Polythioarylenes
Polyacrylics	Polycarboranes	Polyoxyarylenes	Polythioethers
Polyalkenyls	Polycarbosilanes	Polyoxymethylenes	Polythiomethylenes
Polyalkylenes	Polycyanurates	Polyoxyphenylenes	Polythiophenylenes
Polyalkynylenes	Polydienes	Polyphenyls	Polyureas
Polyamic acids	Polyester-polyurethanes	Polyphosphazenes	Polyurethanes
Polyamides	Polyesters	Polypyrroles	Polyvinyl acetals
Polyamincs	Polyetheretherketones	Polypyrrones	Polyvinyl butyrals
Polyanhydrides	Polyether-polyurethanes	Polyquinolines	Polyvinyl formals
Polyarylenealkenylenes	Polyethers	Polyquinoxalines	Vinyl polymers
Polyarylenealkylenes	Polyhydrazides	Polysilanes	

### D. References and Notes

1. IUPAC recommends that subscripts "n" and "x", denoting multiplicities of polymeric sequences, should be italicized, or (in the absence of italics), underlined.
2. Unfortunately the word "copolymer" is used also to indicate a polymer containing two types of monomer. Use of the word "bipolymer" for a polymer containing two types of monomer would be in accord with use of "terpolymer" for a polymer containing three types of monomer, "quaterpolymer" (rather than tetrapolymer) for a polymer containing four types of monomer, etc.
3. IUPAC: "Source-Based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies (Recommendations 1997)." *Pure Appl. Chem.*, 1997, 69, 2511-2521.
4. IUPAC: "Nomenclature of Regular Single-Strand Organic Polymers (Recommendations 1975)." *Pure Appl. Chem.*, 1976, 48, 373-385; reprinted as chapter 5 in ref. 18.

5. Chemical Abstracts Service, 2540 Olentangy River Road, P.O. Box 3012, Columbus, OH 43210: *CA Index Guide*, Appendix IV: Chemical Substance Index Names (© 1999). Section 222 – Description of Polymer Indexing Rules.
6. IUPAC: "Nomenclature of Regular Double-Strand (Ladder and Spiro) Organic Polymers (Recommendations 1993)." *Pure Appl. Chem.*, **1993**, *65*, 1561-1580.
7. Concerning ring seniority, there is one difference between the IUPAC recommendations and the CAS principles: everything else being equal, IUPAC prefers a fused ring system to a spiro ring system, whereas CAS prefers a spiro ring system to a fused ring system. The reason for this one difference is unknown.
8. This name corresponds strictly to a polymer composed entirely of  $-O-CH(Me)-CH_2-$  units. For this polymer, frequently called simply "polyoxypropylene", CAS uses a different approach to registration; in recognition of the occurrence within the polymer of both  $-O-CH(Me)-CH_2-$  and  $-O-CH_2-CH(Me)-$  units, CAS names it poly[oxy(methyl-1,2-ethanedyl)], and the accompanying structure reflects the unspecified position of the methyl group. For the subunit  $-CH_2-CH_2-$ , CAS uses 1,2-ethanedyl, whereas IUPAC permits ethane-1,2-diyl but still prefers ethylene.
9. IUPAC: "Structure-Based Nomenclature for Irregular Single-Strand Organic Polymers (Recommendations 1994)." *Pure Appl. Chem.*, **1994**, *66*, 872-889.
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11. The so-called 9CI nomenclature was introduced by CAS at the beginning of the Ninth Collective Index period (1972). The reasons for its introduction were delineated in the Ninth Collective *CA Index Guide* and in a journal article (see ref. 12).
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17. IUPAC: "Source-Based Nomenclature for Copolymers (Recommendations 1985)." *Pure Appl. Chem.*, **1985**, *57*, 1427-1440; reprinted as chapter 7 in ref. 16.
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19. American Chemical Society: "A Structure-Based Nomenclature for Linear Polymers." *Macromolecules* **1968**, *1*, 193-198.
20. American Chemical Society: "A Structure-Based Nomenclature for Linear Polymers." *Polym. Prepr.*, **1967**, *8*(2), c-r.
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## Alkoxy group

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(Redirected from Alkoxy)

In chemistry, the **alkoxyl** group is an alkyl group linked to oxygen thus: R-O-

In this function, R represents the alkyl group.

An example would be the methoxy group CH<sub>3</sub>O-

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## alkoxy

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alkoxy (al'kāk·sē)

*(organic chemistry)* An alkyl radical attached to a molecule by oxygen, such as the ethoxy radical.Or did you mean: [alkoxy group](#)[Post a question](#) to the [WikiAnswers](#) Community.Get the FREE Answers.com IE Toolbar! [Download Now](#) [More Info](#)Add Answers to the IE7 Toolbar Search Box! [Add Now!](#)

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In chemistry, the **alkoxyl** group is an alkyl group linked to oxygen thus: R-O-

In this function, R represents the alkyl group.

An example would be the methoxy group  $\text{CH}_3\text{O}^-$ , likewise **sodium ethoxide** is the sodium salt of ethanol  $\text{CH}_3\text{CH}_2\text{O}^-\text{Na}^+$ .

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Science > Sci-Tech Dictionary



## hydrosilylation

(|hīdrō'silē'āshən)

*(organic chemistry)* The addition of a Si-H bond to a C-C double bond of an olefin.

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hydrosilylation

Find

Silyl hydrides can even take up the reduction of robust molecules such as carbon dioxide (to methane) [10].

Although it takes a very complex catalyst system.

## Hydrosilylation

Silyl hydrides react with various unsaturated substrates such as alkenes, alkynes, imines, carbonyls and oximes to new organosilicon compounds in **hydrosilylation**. In the reaction of *triphenylsilyl hydride* with phenylacetylene the reaction product is a trans or cis or the geminal vinyl silane, for example [11]:

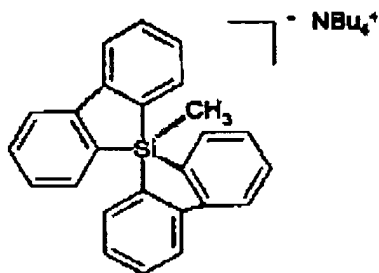
In the related silylmatalation, a metal replaces the hydrogen atom.

## Silenes

Organosilicon compounds unlike their carbon counterparts do not have a rich double bond chemistry due to the large difference in electronegativity. Existing compounds with organosilene Si=C bonds are laboratory curiosities such as the silicon benzene analogue silabenzene, and Si=Si bond containing disilenes.

## Hypercoordinated silicon

Unlike carbon, silicon compounds can be coordinated to five atoms as well in a group of compounds ranging from so-called silatranes to a uniquely stable pentaorganosilicate [12]:



## See also

- Compounds of carbon with period 3 elements: organoaluminum compounds, **organosilicon compounds**, organophosphorus compounds, organosulfur compounds,
- Compounds of carbon with other group 14 elements: **organosilicon compounds**, organogermanium compounds, organotin compounds, organolead compounds.

[CH]